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PLASTIC FLOW STUDIED BY NONEQUILIBRIUM MOLECULAR DYNAMICS COMPUTER SIMULATION

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ABSTRACT

The embedded atom method is adapted to study the plastic flow behavior of a model metal. The elastic properties of real metals are reproduced by a set of basic model potentials as revealed by analytic considerations. NonEquilibrium Molecular Dynamics NEMD computer simulations are performed to study the dynamics and structural changes of the model metal undergoing shear and elongation. The simulations offer insight into the plastic behavior of the model which is used, e.g., to interpret solid friction between metals.

KEYWORDS: PLASTIC FLOW, METAL, EMBEDDED ATOMS, MOLECULAR DYNAMICS

INTRODUCTION

When metal is subjected to stress, it responds by deforming. If only small stresses are applied, then the material returns to its original shape when stress is relieved. In this regime, metals are elastic, if however, the stress exceeds a threshold, then the metal suffers permanent plastic deformation. Physically realistic continuum models of dynamic plasticity are necessarily complicated. The kinematics of a three-dimensional continuum, the thermodynamics of materials, and the physics of microscopic defects enter the description of plastic phenomena. A principal feature of plastic behavior is irrecoverable deformation. On a microscopic level, this behavior is caused by defects in the atomic formation of dislocations. Plastic behavior at the continuum level involves phenomena at different length scales, e.g., interaction of dislocations, dislocation pile-up at grain boundaries, polycrystallinity, anisotropy. A general thermodynamic treatment of phenomenological models has been given, e.g., by Green and Naghdi [1].

In this note we report about preliminary results obtained for a model metal subjected to shear. The model is completely determined by a set of model potentials for N particles, as described in the next section, and it is solved without approximations with computational effort of order N . The results reveal the influence of initial crystal orientation on transient flow behaviors, the formation of shear bands and dislocations, and the general rate-dependence of plastic flow in the strong flow regime. A slightly extended model has been previously applied [2] to a process of solid friction between two metals. As proposed in [2], a profile unbiased temperature control mechanism [3] is used here.

THE EMBEDDED ATOMS METHOD

In order to study plastic deformation and flow of metals we adapted the embedded atom method in the spirit Holian et al. [5]. The method was originated by Daw and Baskes [6], and resembles the fact that in metals the conduction electrons are not localized about the nuclei; the energy depends upon the local electron density, resulting in forces between ions that are many body in character, rather than simply pairwise additive. Accordingly one considers two contributions to the potential energy E of the whole system made up by N particles. There is a conventional binary interaction term through a two-body interaction potential Φ as function of the distance between interaction sites and a term stemming from an embedding functional \mathcal{F} , which produces the effect of the electronic ‘glue’ between atoms

$$E_b = N e_b = \sum_{i=1}^N \left(\frac{1}{2} \sum_{j \neq i}^N \Phi(\mathbf{r}^{ij}) + \mathcal{F}(\rho_i) \right), \quad (1)$$

where $e_b = E_b/N$ represents a ‘binding energy’ per particle. The quantity \mathcal{F} is a nonlinear function of the (local) embedding density ρ_i of atoms $i = 1, \dots, N$. It is constructed from the radial coordinates of surrounding particles and requires the choice of a weighting function $w(r)$: $\rho_i = \sum_j w(\mathbf{r}^{ij}) = w(0) + \sum_{j \neq i} w(\mathbf{r}^{ij})$, where $\mathbf{r}^{ij} \equiv \mathbf{r}^i - \mathbf{r}^j$ is the relative position vector between particle coordinates \mathbf{r}^i and \mathbf{r}^j . Parts of \mathcal{F} linear in ρ_i can be combined with the original repulsive two-particle potential to an effective potential Φ used here which has also an attractive part.

MODEL METAL

A simple choice for the model functions Φ , w and \mathcal{F} leads to our generic model metal, called EMB. For the binary potential function Φ we set $\Phi(r) = \phi_0 r_0^{-4} [3(h-r)^4 - 4(h-r_{min})(h-r)^3]$, $r \leq h$, with an energy scale ϕ_0 , a length scale r_0 , and an interaction range h . The minimum of the potential is located at the distance $r = r_{min} = 2^{1/6} r_0 \approx 1.123 r_0$ as for a Lennard-Jones potential and the well depth of the potential is: $-\Phi(r_{min}) = \phi_0 r_0^{-4} (h - r_{min})^4$. For reasons discussed in [5,7] we use Lucy’s weight function $w(r) = w_0 (1 + 3r/h) (1 - r/h)^3$ for $r \leq h$ normalized to unity (via w_0).

The particular simple parabolic embedding potential for EMB is

$$\mathcal{F}(\rho) = F_0 \phi_0 r_0^6 ((\rho - \rho_0)^2 - (w_0 - \rho_0)^2) + \dots, \quad (2)$$

where ρ_0 is the desired embedding number density and F_0 is the embedding strength; the dots denote higher order terms in $(\rho - \rho_0)$ which may be considered in order to obtain more than a qualitative agreement between theory and experiments with respect to the quantities listed in Tab. 1. Throughout this work we investigate the ‘basic’ model metal for which the desired density $\rho_0 = r_0^{-3}$ equals the particle number density $n \equiv N/V = r_0^{-3}$; $h = 1.6 r_0$ and the temperature $k_B T = 0.01 \phi_0$ are fixed.

REFERENCE QUANTITIES AND ELASTIC PROPERTIES OF EMB

To compare with experimental data one has to estimate reference values for dimensionless simulation quantities, which may be expressed in terms of reduced units for length $r_{\text{ref}} = r_0$, energy $e_{\text{b,ref}} = \phi_0 = k_B T_{\text{ref}}$ pressure $P_{\text{ref}} = \phi_0 r_0^{-3} = r_0^{-3} e_{\text{b,ref}}$, or time $t_{\text{ref}} = r_0 (m/e_{\text{b,ref}})^{1/2}$. for which experimental values are available. For Ag, e.g., one obtains model parameters $r_0 = n_{\text{ref}}^{-1/3} = 2.56 \text{ \AA}$, $\phi_0 = 47.4 \cdot 10^{-18} \text{ J}$ and $m = 107.8 \text{ g/mol}$.

metal	n_{ref}	T_{ref}	P_{ref}	E	G	c_{ani}
Ag	59.4	34.3	28	101	38	2.99
Cu	85.5	40.6	48	156	59	3.19
EMB	72.5	40.0	40	260	95	2.56
Fe	85.2	49.8	59	232	94	2.32
Ni	92.0	51.8	65	239	101	2.39

Tab. 1. Reference values for a set of metals, including the model metal EMB ($n = 1$, $F_0 = 1$), together with reported values for the elastic (E) and shear (G) moduli and the elastic anisotropy. The coefficients c_{ij} denote Voigt moduli [4]. n_{ref} in nm^{-3} , T_{ref} in 1000K, P_{ref} and elastic moduli in GPa; $c_{\text{ani}} \equiv 2c_{44}/(c_{11} - c_{12})$.

NEMD COMPUTER SIMULATION: METHOD AND RESULTS

The equations of motions were integrated by a velocity-Verlet algorithm as in [5]. The parameters h, T, ρ_0 and the average particle density $n = N/V$ were fixed by the model. The influence of the embedding functional \mathcal{F} can be estimated by varying its strength F_0 . A flow simulation introduces further independent variables, which describe the geometry and strength of flow. Details of a NEMD simulation algorithm, the implementation of Lees-Edwards boundary conditions and periodic images see, e.g. [8]. In the simulations the stress tensor is obtained from the tensorial virial expression.

A. Shear flow

Figure 1 shows a time series for a subsystem of a cubic cell with $N = 60000$ particles undergoing shear at intermediate rate, c.f., Fig. 3-4 which report about transient and stationary rheological and structural behaviors. Three time series for a smaller system with $N = 2048$ particles are shown in Fig. 2. At low rates shear bands are observed, at intermediate rates fluid and crystalline domains coexist and the metal is of course partially molten at the the highest rate which corresponds, for Ag, to a real relative velocity of about 100 m/s between atomic layers.

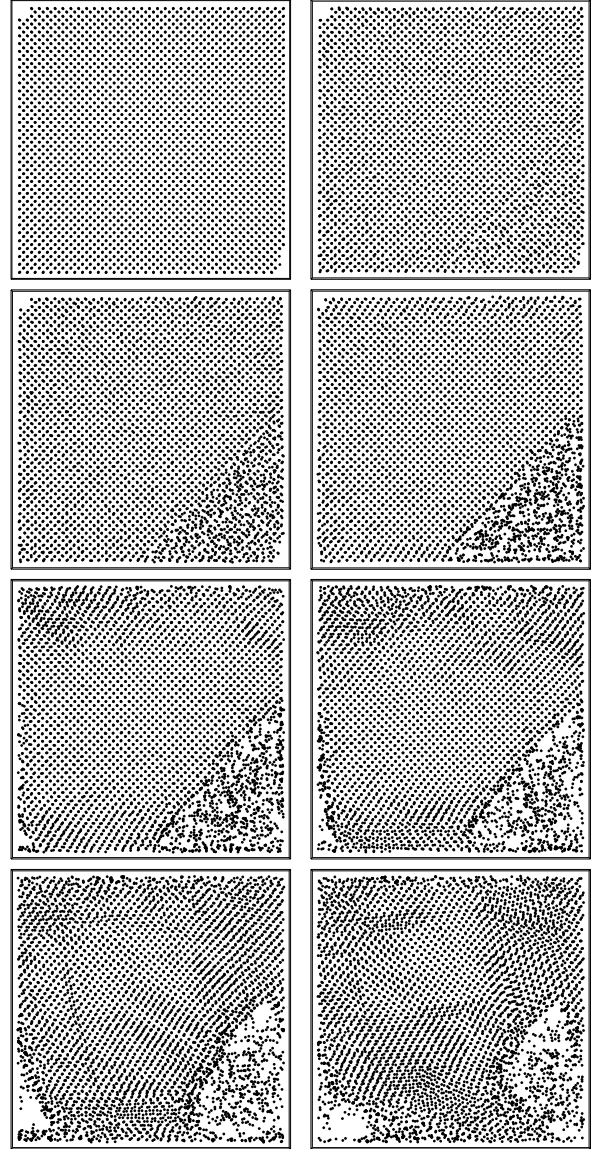
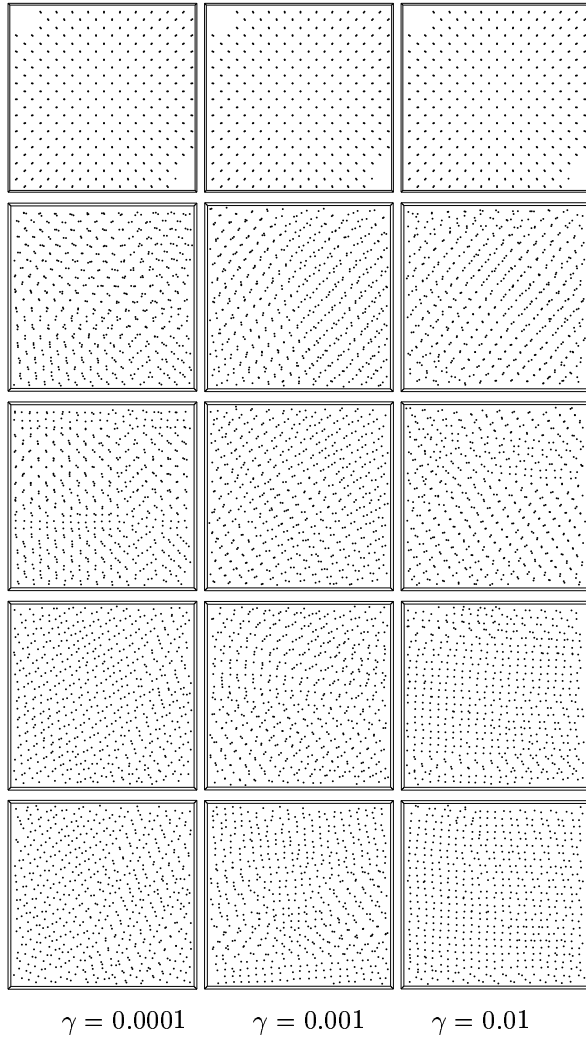


Fig. 1. Particle positions at times $t = 0.5$ (top left), 1, 2, 5, 10, 25, 50, 100, 200 (bottom right) for the model metal EMB undergoing shear with shear rate $\gamma = 0.01$.



$\gamma = 0.0001$ $\gamma = 0.001$ $\gamma = 0.01$

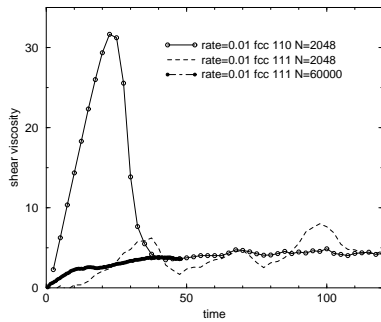


Fig. 3a. Transient shear viscosity vs time for EMB at different initial conditions and systems sizes N .

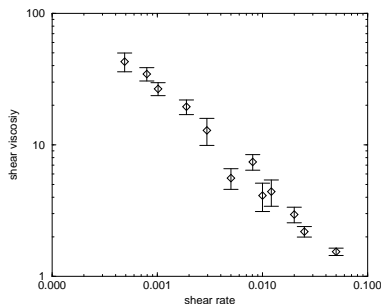


Fig. 3b. Shear viscosity vs shear rate for EMB obtained in the stationary flow regime.

(left) Fig. 2. The model metal EMB undergoing shear at constant rate γ . A selected number of particle positions (a layer with thickness 3 within the shearing plane) is shown in the snapshots. From top to bottom the time t (\propto strain) is increasing in equidistant steps. Strain at bottom is $\gamma t = 2.5$. For every column, the shear rate γ is given in the figure.

B. Uniaxial compression

The model metal is uniaxially compressed at constant elongation rate. We observe spontaneous symmetry breaking. The often quoted ‘theoretical value’ for the critical penetration hardness σ_c should be $\sigma_c = cG$ with the shear modulus G and $c = c_{\text{theo}} = 1/10$. The experimentally observed factor is smaller, $c_{\text{exp}} = 10^{-3} - 10^{-2}$. Our preliminary result is $c_{\text{sim}} \approx 1/50$ being estimated from the simulated normal pressure p_{yy} .

CONCLUSIONS

The embedded atom method has been adapted to study the mechanical behavior of the model metal EMB. The elastic properties of real metals are reproduced by a set of basic model potentials. NEMD computer simulations are performed to study the dynamics and structural changes of the model metal undergoing a shear and uniaxial compression in order to analyze the formation of transient structures and plastic yield. Longer simulation runs are needed to determine values for the penetration hardness with high precision. Variants of the model metal EMB should be characterized.

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